Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1129pxo

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	18	FEB 10	STN Patent Forums to be held in March 2005
NEWS	19	FEB 16	STN User Update to be held in conjunction with the 229th ACS National Meeting on March 13, 2005
NEWS	20	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	21	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	22	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	23	MAR 02	GBFULL: New full-text patent database on STN
NEWS	24	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	25	MAR 03	MEDLINE file segment of TOXCENTER reloaded

NEWS EXPRESS	JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:45:11 ON 18 MAR 2005

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.63	0.63

FILE 'REGISTRY' ENTERED AT 14:47:12 ON 18 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 MAR 2005 HIGHEST RN 845858-62-0
DICTIONARY FILE UPDATES: 17 MAR 2005 HIGHEST RN 845858-62-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10677288c.str

L1 STRUCTURE UPLOADED

=> s l1
STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large. You may delete attributes or atoms to reduce the size of the structure and try again.

=>
Uploading C:\Program Files\Stnexp\Queries\10677288e.str

L2 STRUCTURE UPLOADED

=> s l2
STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large. You may delete

```
attributes or atoms to reduce the size of the structure
and try again.

=>
Uploading C:\Program Files\Stnexp\Queries\10677288f.str

L3      STRUCTURE UPLOADED

=> s l3
SAMPLE SEARCH INITIATED 14:52:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   2763 TO ITERATE

 36.2% PROCESSED    1000 ITERATIONS                                 1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        52108 TO    58412
PROJECTED ANSWERS:               1 TO      154

L4            1 SEA SSS SAM L3

=> search l3
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:52:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  56351 TO ITERATE

100.0% PROCESSED   56351 ITERATIONS                              47 ANSWERS
SEARCH TIME: 00.00.01

L5           47 SEA SSS FUL L3

=>
Uploading C:\Program Files\Stnexp\Queries\10677288g.str

L6      STRUCTURE UPLOADED

=> s l6
STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large.  You may delete
attributes or atoms to reduce the size of the structure
and try again.

=>
Uploading C:\Program Files\Stnexp\Queries\10677288h.str

L7      STRUCTURE UPLOADED

=> s l7
STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large.  You may delete
attributes or atoms to reduce the size of the structure
and try again.

=>
Uploading C:\Program Files\Stnexp\Queries\10677288i.str

L8      STRUCTURE UPLOADED
```

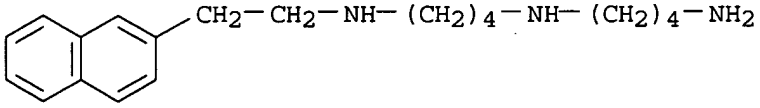
```
=> s l8
STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large.  You may delete
attributes or atoms to reduce the size of the structure
and try again.

=>
Uploading C:\Program Files\Stnexp\Queries\10677288j.str

L9      STRUCTURE UPLOADED

=> s l9
STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large.  You may delete
attributes or atoms to reduce the size of the structure
and try again.

=>
Uploading C:\Program Files\Stnexp\Queries\10677288k.str

L10     STRUCTURE UPLOADED

=> d l10
L10 HAS NO ANSWERS
L10             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l10
STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large.  You may delete
attributes or atoms to reduce the size of the structure
and try again.

=>
Uploading C:\Program Files\Stnexp\Queries\10677288l.str

L11     STRUCTURE UPLOADED

=> s l11
SAMPLE SEARCH INITIATED 15:08:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1859 TO ITERATE

 53.8% PROCESSED    1000 ITERATIONS                                1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        34594 TO    39766
PROJECTED ANSWERS:               1 TO      118

L12           1 SEA SSS SAM L11

=> search l11
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
```

```
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 15:08:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  38377 TO ITERATE

100.0% PROCESSED   38377 ITERATIONS                          15 ANSWERS
SEARCH TIME: 00.00.01

L13          15 SEA SSS FUL L11

=> d his

     (FILE 'HOME' ENTERED AT 14:45:11 ON 18 MAR 2005)

     FILE 'REGISTRY' ENTERED AT 14:47:12 ON 18 MAR 2005
L1              STRUCTURE UPLOADED
L2              STRUCTURE UPLOADED
L3              STRUCTURE UPLOADED
L4            1 S L3
L5           47 SEARCH L3 FULL
L6              STRUCTURE UPLOADED
L7              STRUCTURE UPLOADED
L8              STRUCTURE UPLOADED
L9              STRUCTURE UPLOADED
L10             STRUCTURE UPLOADED
L11             STRUCTURE UPLOADED
L12           1 S L11
L13          15 SEARCH L11 FULL

=> s l5 or l13
L14         47 L5 OR L13

=> file caplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                               ENTRY    SESSION
FULL ESTIMATED COST                           337.28     337.91

FILE 'CAPLUS' ENTERED AT 15:08:55 ON 18 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 18 Mar 2005  VOL 142 ISS 13
FILE LAST UPDATED: 17 Mar 2005  (20050317/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l14
```

L15 13 L14

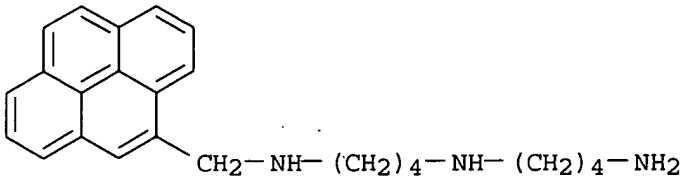
=> d l15 fbib ab hitstr 1-13

L15 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:861007 CAPLUS
DN 142:32437
TI N1-Substituent Effects in the Selective Delivery of Polyamine Conjugates into Cells Containing Active Polyamine Transporters
AU Gardner, Richard Andrew; Delcros, Jean-Guy; Konate, Fanta; Breitbeil, Fred, III; Martin, Benedicte; Sigman, Michael; Huang, Min; Phanstiel, Otto, IV
CS Department of Chemistry, University of Central Florida, Orlando, FL, 32816-2366, USA
SO Journal of Medicinal Chemistry (2004), 47(24), 6055-6069
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB Several N1-arylalkylpolyamines containing various aromatic ring systems were synthesized as their resp. HCl salts. The N1-substituents evaluated ranged in size from N1-benzyl, N1-naphthalen-1-ylmethyl, N1-2-(naphthalen-1-yl)ethyl, N1-3-(naphthalen-1-yl)propyl, N1-anthracen-9-ylmethyl, N1-2-(anthracen-9-yl)ethyl, N1-3-(anthracen-9-yl)propyl, and pyren-1-ylmethyl. The polyamine architecture was also altered and ranged from diamine to triamine and tetraamine systems. Biol. activities in L1210 (murine leukemia), Chinese hamster ovary (CHO), and CHO's polyamine transport-deficient mutant (CHO-MG) cell lines were investigated via IC50 cytotoxicity detns. Ki values for spermidine uptake were also determined in L1210 cells. The size of the N1-arylalkyl substituent as well as the polyamine sequence used had direct bearing on the observed cytotoxicity profiles. N1-Tethers longer than ethylene showed dramatic loss of selectivity for the polyamine transporter (PAT) as shown in a CHO/CHO-MG cytotoxicity screen. In summary, there are clear limits to the size of N1-substituents, which can be accommodated by the polyamine transporter. A direct correlation was observed between polyamine-conjugate uptake and cytotoxicity. In this regard, a cytotoxicity model was proposed, which describes a hydrophobic pocket of set dimensions adjacent to the putative PAT polyamine-binding site.
IT **805229-80-5P**
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(N1-substituent effects in selective delivery of polyamine conjugates into cells containing active polyamine transporters)
RN 805229-80-5 CAPLUS
CN 1,4-Butanediamine, N-(4-aminobutyl)-N'-[2-(2-naphthalenyl)ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

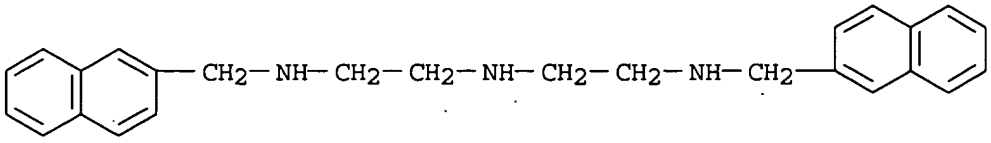
IT **805229-79-2**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(N1-substituent effects in selective delivery of polyamine conjugates into cells containing active polyamine transporters)
RN 805229-79-2 CAPLUS
CN 1,4-Butanediamine, N-(4-aminobutyl)-N'-(4-pyrenylmethyl)-, trihydrochloride (9CI) (CA INDEX NAME)



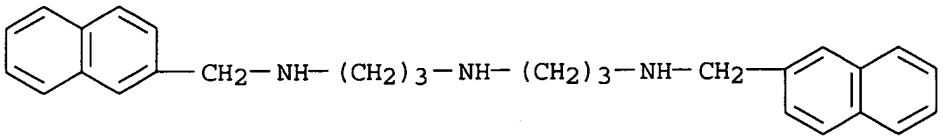
● 3 HCl

RE.CNT 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:606913 CAPLUS
DN 141:310543
TI Self-organization of oligomeric helical stacks controlled by substrate binding in a tobacco mosaic virus like self-assembly process
AU Petitjean, Anne; Nierengarten, Helene; van Dorosselaer, Alain; Lehn, Jean-Marie
CS Laboratoire de Chimie Supramoleculaire, ISIS, Strasbourg, BP 70028, Fr.
SO Angewandte Chemie, International Edition (2004), 43(28), 3695-3699
CODEN: ACIEF5; ISSN: 1433-7851
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
AB Self-assembly with a twist: Linear polyammonium threads are templates in the organization of helical heterocyclic building blocks to form stacks of helixes as a model for the Tobacco Mosaic Virus. The length of the cationic substrate and the spacing of the pos. charges within the thread dictate the size of the final self-organized supramol. architecture.
IT **176977-11-0 767330-07-4 767330-09-6**
RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); BIOL (Biological study); PROC (Process)
(modeling of tobacco mosaic virus self-assembly through self-organization of oligomeric helical stacks of organic compds.)
RN 176977-11-0 CAPLUS
CN 1,2-Ethanediamine, N-(2-naphthalenylmethyl)-N'-[2-[(2-naphthalenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

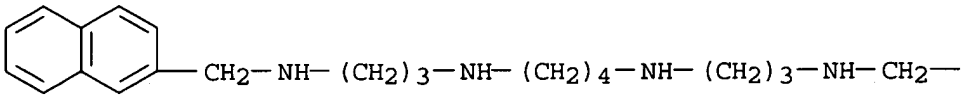


RN 767330-07-4 CAPLUS
CN 1,3-Propanediamine, N-(2-naphthalenylmethyl)-N'-[3-[(2-naphthalenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

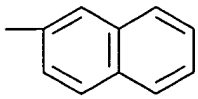


RN 767330-09-6 CAPLUS
CN 1,4-Butanediamine, N,N'-bis[3-[(2-naphthalenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



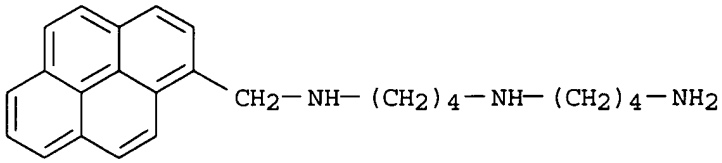
RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:827041 CAPLUS
DN 140:35486
TI Defining the Molecular Requirements for the Selective Delivery of Polyamine Conjugates into Cells Containing Active Polyamine Transporters
AU Wang, Chaojie; Delcros, Jean-Guy; Cannon, Laura; Konate, Fanta; Carias, Horacio; Biggerstaff, John; Gardner, Richard Andrew; Phanstiel, Otto
CS Groupe de Recherche en Therapeutique Anticancereuse, Faculte de Medecine, University of Rennes 1, Rennes, 35043, Fr.
SO Journal of Medicinal Chemistry (2003), 46(24), 5129-5138
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB Several N1-substituted polyamines containing various spacer units between nitrogen centers were synthesized as their resp. HCl salts. The N1-substituents included benzyl, naphthalen-1-ylmethyl, anthracen-9-ylmethyl, and pyren-1-ylmethyl. The polyamine spacer units ranged from generic (4,4-triamine, 4,3-triamine, and diaminooctane) spacers to more exotic [2-(ethoxy)ethanoxy-containing diamine, hydroxylated 4,3-triamine, and cyclohexylene-containing triamine] spacers. Two control compds. were also evaluated:N-(anthracen-9-ylmethyl)-butylamine and N-(anthracen-9-ylmethyl)-butanediamine. Biol. activities in L1210 (murine

leukemia), α-difluoromethylornithine (DFMO)-treated L1210, and Chinese hamster ovary (CHO) and its polyamine transport-deficient mutant (CHO-MG) cell lines were investigated via IC50 cytotoxicity detns. Ki values for spermidine uptake were also determined in L1210 cells. Of the series studied, the N1-benzyl-4,4-triamine derivative (6) had significantly higher IC50 values (lower cytotoxicity) in the L1210, CHO, and CHO-MG cell lines. A cellular debenzylation process was observed in L1210 cells with 6 and generated "free" homospermidine. The size of the N1-arylmethyl substituent had direct bearing on the observed cytotoxicity in CHO-MG cells. The N1-naphthalenylmethyl, N1-anthracenylmethyl, and N1-pyrenylmethyl 4,4-triamines had similar toxicity (IC50s: .apprx.0.5 μM) in CHO cells, which have an active polyamine transporter (PAT). However, this series had IC50 values of >100 μM, 66.7 μM, and 15.5 μM, resp., in CHO-MG cells, which are PAT-deficient. The observed lower cytotoxicity in the PAT-deficient CHO-MG cell line supported the premise that the conjugates use PAT for cellular entry. In general, moderate affinities for the polyamine transporter were observed for the N-arylmethyl 4,4-triamine series with their L1210 Ki values all near 3 μM. In summary, the 4,4-triamine motif was shown to facilitate entry of polyamine conjugates into cells containing active polyamine transporters.

IT **635304-07-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(defining the mol. requirements for selective delivery of polyamine conjugates into cells containing active polyamine transporters)

RN 635304-07-3 CAPLUS
CN 1,4-Butanediamine, N-(4-aminobutyl)-N'-(1-pyrenylmethyl)-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

RE.CNT 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:477826 CAPLUS
DN 137:262736
TI Open-chain polyazaalkanes functionalised with pyrene groups as sensing fluorogenic receptors for metal ions
AU Sancenon, Felix; Descalzo, Ana Belen; Lloris, Jose Manuel; Martinez-Manez, Ramon; Pardo, Teresa; Segui, Maria Jesus; Soto, Juan
CS Departamento de Quimica, Universidad Politecnica de Valencia, Valencia, 46071, Spain
SO Polyhedron (2002), 21(14-15), 1397-1404
CODEN: PLYHDE; ISSN: 0277-5387
PB Elsevier Science Ltd.
DT Journal
LA English

OS CASREACT 137:262736

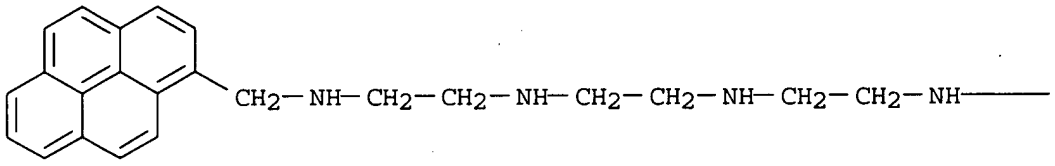
AB The new open-chain polyazaalkanes ligands (I; R = H, CH2-pyrenyl, CH2CH2NH2, CH2CH2NH-pyrenyl, L1-L4) functionalized with one or two pyrene groups were synthesized and characterized and their potential use as selective cation and anion sensing chemosensors studied. Solution studies by potentiometric methods were carried out in the presence of Cu2+ and Zn2+ in MeCN-H2O (70:30 volume/volume, 0.1 mol dm-3 Bu4NClO4, 25°) and the results are compared with those reported for the analogous nonfunctionalized ligand triethylentetraamine (tta). The fluorescence behavior of the ligands L1-L4 was studied as a function of the pH in the presence of the metal cations Ni2+, Cu2+, Zn2+, Cd2+, Hg2+ and Pb2+ in MeCN-H2O 70:30 volume/volume mixts. The Zn2+ and Cd2+ cations enhance the fluorescence emission of the L1-L4 chemosensors at basic pH, whereas Cu2+ induce quenching of the fluorescence emission at acid pH. The fluorescence behavior of L1-L4 receptors was also studied as a function of the pH in MeCN-H2O 70:30 volume/volume in the presence of anions.

IT **461668-36-0P 461668-37-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and fluorescence with and without transition metal ions)

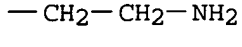
RN 461668-36-0 CAPLUS

CN 1,2-Ethanediamine, N-[2-[(2-aminoethyl)amino]ethyl]-N'-[2-[(1-pyrenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



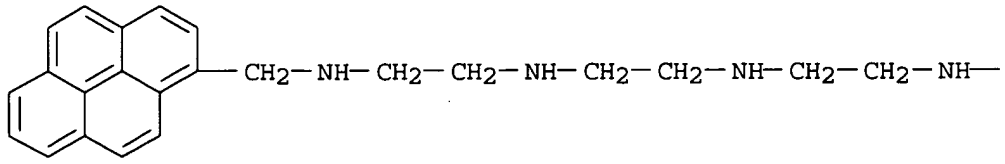
PAGE 1-B



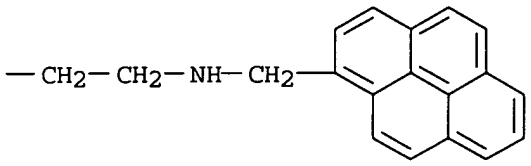
RN 461668-37-1 CAPLUS

CN 1,2-Ethanediamine, N-[2-[(1-pyrenylmethyl)amino]ethyl]-N'-[2-[[2-[(1-pyrenylmethyl)amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

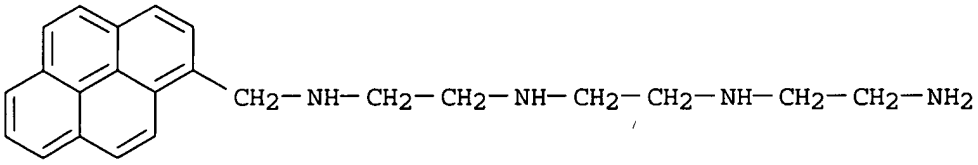
PAGE 1-A



PAGE 1-B



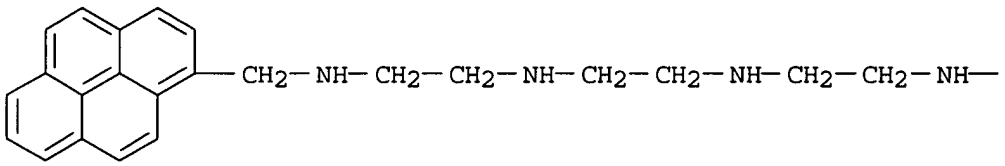
IT **461668-30-4P 461668-31-5P 461668-32-6P**
461668-33-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 461668-30-4 CAPLUS
CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-[2-[(1-pyrenylmethyl)amino]ethyl]-, tetrahydrochloride (9CI) (CA INDEX NAME)



● 4 HCl

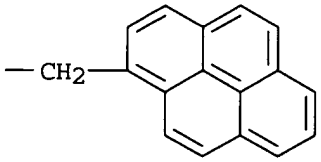
RN 461668-31-5 CAPLUS
CN 1,2-Ethanediamine, N,N'-bis[2-[(1-pyrenylmethyl)amino]ethyl]-, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



● 4 HCl

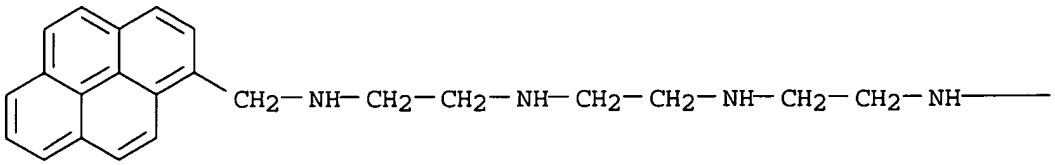
PAGE 1-B



RN 461668-32-6 CAPLUS

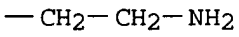
CN 1,2-Ethanediamine, N-[2-[(2-aminoethyl)amino]ethyl]-N'-[2-[(1-pyrenylmethyl)amino]ethyl]-, pentahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



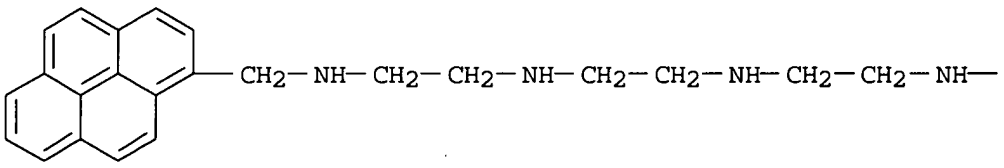
●5 HCl

PAGE 1-B



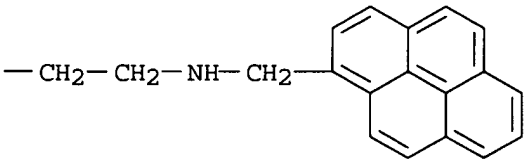
RN 461668-33-7 CAPLUS
CN 1,2-Ethanediamine, N-[2-[(1-pyrenylmethyl)amino]ethyl]-N'-[2-[[2-[(1-pyrenylmethyl)amino]ethyl]amino]ethyl]-, pentahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



●5 HCl

PAGE 1-B

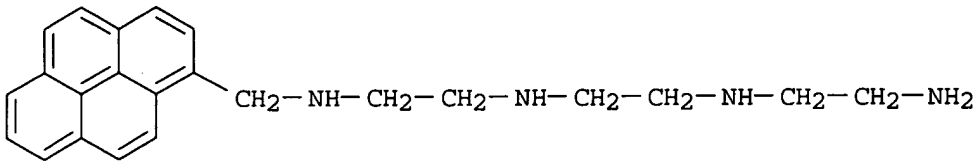


IT **461668-34-8P 461668-35-9P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, protonation, fluorescence and complexation with copper(II) and zinc)

RN 461668-34-8 CAPLUS

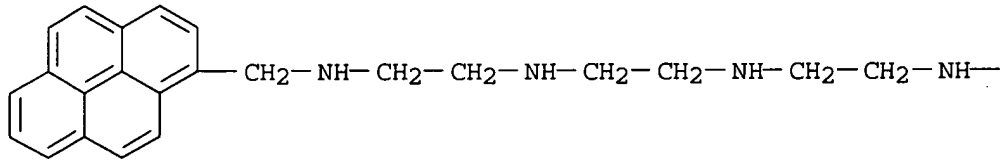
CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-[2-[(1-pyrenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



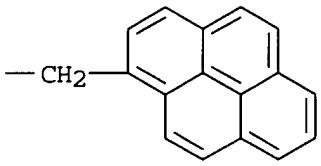
RN 461668-35-9 CAPLUS

CN 1,2-Ethanediamine, N,N'-bis[2-[(1-pyrenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



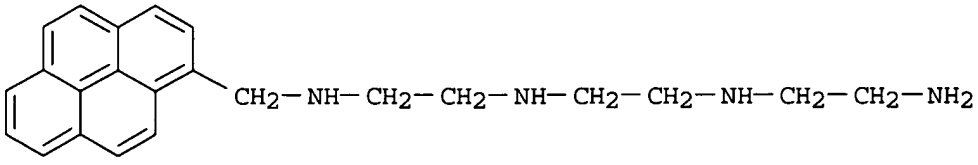
IT **461668-34-8D**, copper complex **461668-35-9D**, copper and zinc complexes

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(stability constant)

RN 461668-34-8 CAPLUS

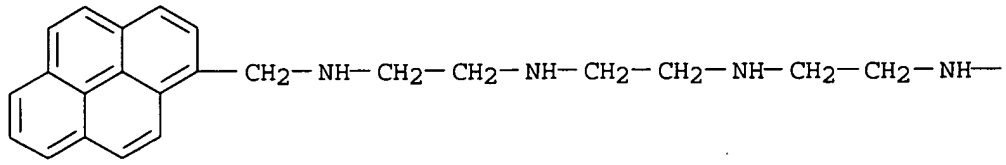
CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-[2-[(1-pyrenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)



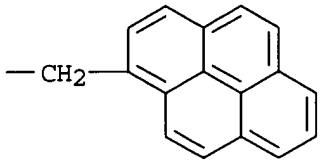
RN 461668-35-9 CAPLUS

CN 1,2-Ethanediamine, N,N'-bis[2-[(1-pyrenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:319661 CAPLUS
DN 134:336203
TI Substituted succinic acid metallo-β-lactamase inhibitors, their preparation, and their use in treating bacterial infections
IN Balkovec, James M.; Greenlee, Mark L.; Olson, Steven H.; Rouen, Gregory P.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
PI	WO 2001030148	A1	20010503	WO 2000-US29707		20001027
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
				US 1999-162370P	P	19991028
	US 6630510	B1	20031007	US 2000-697415		20001026
				US 1999-162370P	P	19991028
	CA 2388076	AA	20010503	CA 2000-2388076		20001027
				US 1999-162370P	P	19991028
				WO 2000-US29707	W	20001027
	EP 1227721	A1	20020807	EP 2000-975454		20001027
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL					
				US 1999-162370P	P	19991028
				WO 2000-US29707	W	20001027
	JP 2003527332	T2	20030916	JP 2001-532588		20001027

			US 1999-162370P	P	19991028
			WO 2000-US29707	W	20001027
AU 771274	B2	20040318	AU 2001-13504		20001027
			US 1999-162370P	P	19991028
			WO 2000-US29707	W	20001027
US 2003078418	A1	20030424	US 2002-99790		20020315
			US 1999-162370P	P	19991028
			US 2000-697415	A3	20001026
US 2003207859	A1	20031106	US 2003-339043		20030109
			US 1999-162370P	P	19991028
			US 2000-697415	A3	20001026

OS MARPAT 134:336203

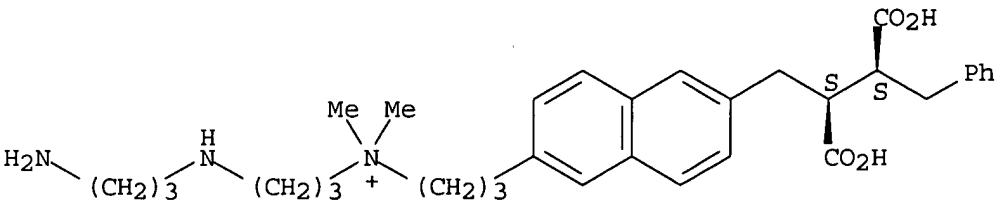
AB Substituted succinic acid metallo-β-lactamase inhibitors are provided which are useful potentiators of β-lactam antibiotics. Accordingly, the invention provides a method of treating bacterial infections in animals or humans which comprises administering, together with a β-lactam antibiotic, a therapeutically effective amount of a succinic acid derivative of the invention, or a pharmaceutically acceptable salt, prodrug, anhydride, or solvate thereof.

IT **337907-35-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(succinic acid derivative metallo-β-lactamase inhibitors, preparation, and use in treating bacterial infections)

RN 337907-35-4 CAPLUS

CN 2-Naphthalenepropanaminium, N-[3-[(3-aminopropyl)amino]propyl]-6-[(2S,3S)-2,3-dicarboxy-4-phenylbutyl]-N,N-dimethyl-, chloride, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Cl⁻

●2 HCl

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

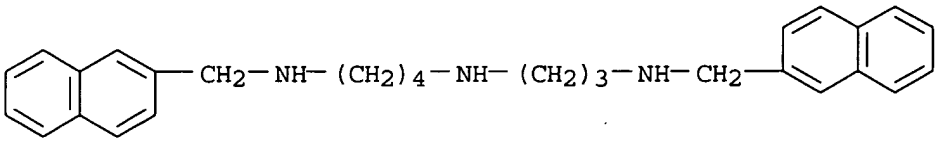
AN 1998:34062 CAPLUS

DN 128:188273

TI Polyamine derivatives as inhibitors of trypanothione reductase and assessment of their trypanocidal activities

AU O'sullivan, Mary C.; Zhou, Qibing; Li, Zhili; Durham, Timothy B.; Rattendi, Donna; Lane, Schennella; Bacchi, Cyrus J.

CS Department of Chemistry, Indiana State University, Terre Haute, IN, 47809, USA
SO Bioorganic & Medicinal Chemistry (1997), 5(12), 2145-2155
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
AB Trypanothione reductase (TR) occurs exclusively in trypanosomes and leishmania, which are the etiol. agents of many diseases. TR plays a vital role in the antioxidant defenses of these parasites and inhibitors of TR have potential as antitrypanosomal agents. We describe the syntheses of several spermine and spermidine derivs. and the inhibiting effects of these compds. on T. cruzi TR. All of the inhibiting compds. displayed competitive inhibition of TR-mediated reduction of trypanothione disulfide. The three most effective compds. studied were N4,N8-bis(3-phenylpropyl)spermine (I), N4,N8-bis(2-naphthylmethyl)spermine (II), and N1,N8-bis(2-naphthylmethyl)spermidine (III), with Ki values of 3.5, 5.5 and 9.5 μM, resp. Compds. I, II, and III were found to be potent trypanocides in vitro with IC50 values ranging from 0.19 to 0.83 μM against four T. brucei ssp. strains. However, these compds. did not prolong the lives of mice infected with trypanosomes. This work indicates that certain polyamine derivs. which target a unique pathway in Trypanosomatidae have potential as antitrypanosomal agents.
IT **168101-39-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of polyamine derivs. as inhibitors of trypanothione reductase and assessment of their trypanocidal activities)
RN 168101-39-1 CAPLUS
CN 1,4-Butanediamine, N-(2-naphthalenylmethyl)-N'-[3-[(2-naphthalenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)



RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

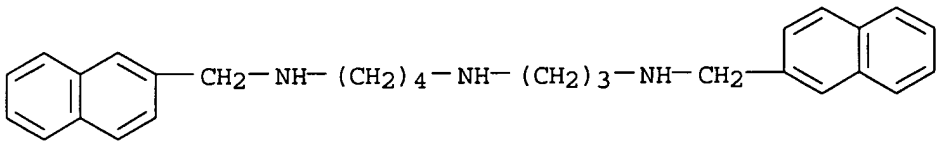
L15 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1997:237990 CAPLUS
DN 127:12989
TI Inhibiting effects of spermidine derivatives on Trypanosoma cruzi trypanothione reductase
AU O'Sullivan, Mary C.; Dalrymple, Damon M.; Zhou, Qibing
CS Department Chemistry, Indiana State University, Terre Haute, IN, 47809, USA
SO Journal of Enzyme Inhibition (1996), 11(2), 97-114
CODEN: ENINEG; ISSN: 8755-5093
PB Harwood
DT Journal
LA English
AB The preparation of several spermidine derivs. is described and their inhibition kinetics in the reduction of trypanothione by Trypanosoma cruzi trypanothione reductase (I) were studied. Spermidine derivs. containing hydrophobic aromatic

substituents were found to be competitive inhibitors of I. N4-acylated spermidine derivs. were less effective inhibitors than the corresponding N4-alkylated derivs. The most effective compds. studied were N1,N8-bis(2-naphthylmethyl)spermidine (II) and N4-(2-naphthylmethyl)spermidine, with Ki values of 9.5 and 108 μM, resp. The results of these studies indicated the relative importance of specific structural features required for spermidine derivs. to be inhibitors of I. The most potent compds. in this study contained naphthyl substituents; compds. with benzyl substituents were less effective inhibitors. Spermidine derivs. such as II are easy to prepare and are inexpensive and thus may provide a new direction for the development of affordable antitrypanosomal agents.

IT **168101-39-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of spermidine derivs. and their inhibition kinetics with Trypanosoma cruzi trypanothione reductase)

RN 168101-39-1 CAPLUS

CN 1,4-Butanediamine, N-(2-naphthalenylmethyl)-N'-[3-[(2-naphthalenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)



L15 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:238014 CAPLUS

DN 125:10253

TI Terminal Alkylation of Linear Polyamines

AU Sclafani, Joseph A.; Maranto, Maria T.; Sisk, Thomas M.; Van Arman, Scott A.

CS Department of Chemistry, Franklin and Marshall College, Lancaster, PA, 17604-3003, USA

SO Journal of Organic Chemistry (1996), 61(9), 3221-2
CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

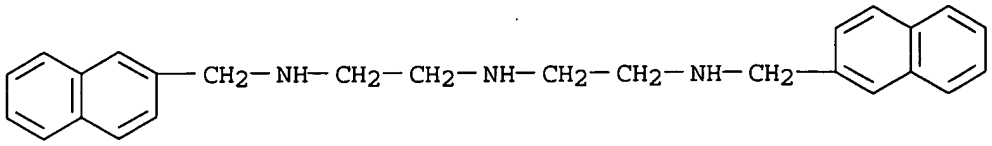
LA English

AB Linear polyamines are known to be interesting agents for a wide variety of reasons. Their synthetic elaboration has been limited but is of fundamental importance. The general use of a simple reductive amination sequence for the selective alkylation of terminal amines in linear polyamines is reported. Yields of up to 73% are reported.

IT **176977-06-3P 176977-07-4P 176977-08-5P**
176977-11-0P 176977-12-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 176977-06-3 CAPLUS

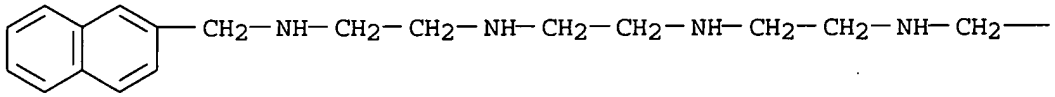
CN 1,2-Ethanediamine, N-(2-naphthalenylmethyl)-N'-[2-[(2-naphthalenylmethyl)amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)



● 3 HCl

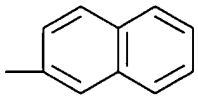
RN 176977-07-4 CAPLUS
CN 1,2-Ethanediamine, N,N'-bis[2-[(2-naphthalenylmethyl)amino]ethyl]-, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



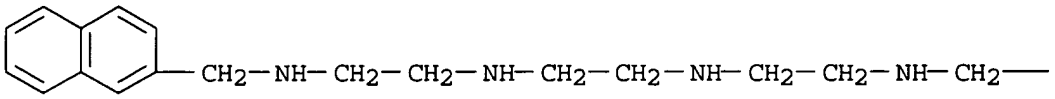
● 4 HCl

PAGE 1-B



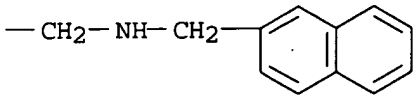
RN 176977-08-5 CAPLUS
CN 1,2-Ethanediamine, N-[2-[(2-naphthalenylmethyl)amino]ethyl]-N'-[2-[[2-[(2-naphthalenylmethyl)amino]ethyl]amino]ethyl]-, pentahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

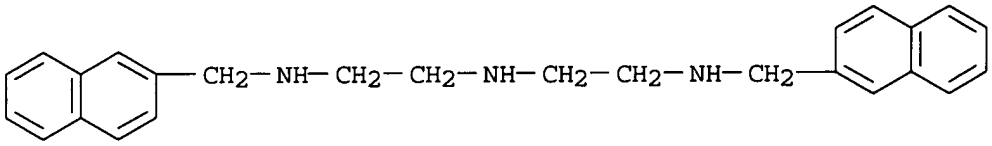


● 5 HCl

PAGE 1-B

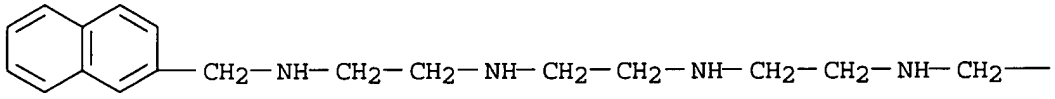


RN 176977-11-0 CAPLUS
CN 1,2-Ethanediamine, N-(2-naphthalenylmethyl)-N'-[2-[(2-naphthalenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

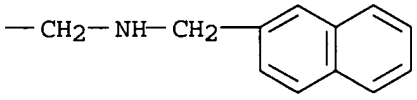


RN 176977-12-1 CAPLUS
CN 1,2-Ethanediamine, N-[2-[(2-naphthalenylmethyl)amino]ethyl]-N'-[2-[[2-[(2-naphthalenylmethyl)amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



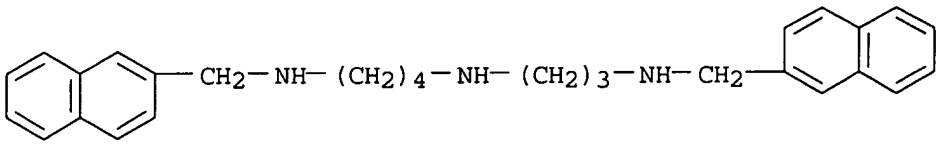
L15 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1995:796292 CAPLUS
DN 123:221529
TI Novel polyamine derivatives as potent competitive inhibitors of Trypanosoma cruzi trypanothione reductase
AU O'Sullivan, Mary C.; Zhou, Qibing
CS Department of Chemistry, Indiana State University, Terre Haute, IN, 47809, USA
SO Bioorganic & Medicinal Chemistry Letters (1995), 5(17), 1957-60
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier
DT Journal
LA English
AB The inhibiting effects of several spermidine and spermine derivs. on T. cruzi trypanothione reductase were assessed. Spermidine and spermine derivs. containing hydrophobic aromatic substituents were competitive inhibitors

of trypanothione reductase. The most effective compds. tested were N1,N8-bis(2-naphthylmethyl)spermidine, N4,N8-bis(2-naphthylmethyl)spermine and N4,N8-bis(3-phenylpropyl)spermine.

IT **168101-39-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(novel polyamine derivs. as potent competitive inhibitors of Trypanosoma cruzi trypanothione reductase)

RN 168101-39-1 CAPLUS

CN 1,4-Butanediamine, N-(2-naphthalenylmethyl)-N'-[3-[(2-naphthalenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)



L15 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:404656 CAPLUS

DN 123:198340

TI Platelet aggregation inhibiting and anticoagulant effects of oligoamines. XXVIII: Oligoamines with fluorescent properties. Part C: Fluorescent oligoamines with enhanced hydrophilic properties

AU Rehse, Klaus; Seidel, Torsten

CS Institut Pharmazie Freie, Universitaet Berlin, Berlin, 14195, Germany

SO Archiv der Pharmazie (Weinheim, Germany) (1995), 328(2), 131-5
CODEN: ARPMAS; ISSN: 0365-6233

PB VCH

DT Journal

LA English

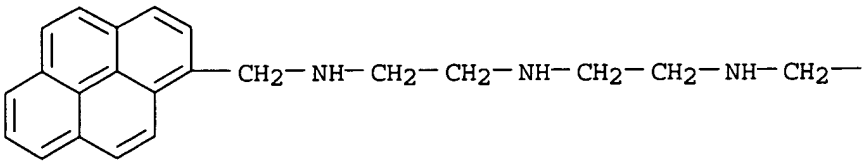
AB Fifteen fluorescent oligoamines with one or two fluorescent groups and two or three basic N-functions were prepared and tested for antiplatelet activity (Born-test). Five compds. involving three different fluorophores, i.e. 2-fluorenyl, 1-pyrenyl, and 9-phenanthryl, show an IC50 of 7-11 μmol/L. They are suitable to serve as probes in the field of oligoamine-biopolymer interactions. An example compound is N-[4-(9H-fluoren-2-yl)butyl]-N'-octyl-1,5-pentanediamine dihydrochloride.

IT **167562-38-1P 167562-39-2P 167562-40-5P**
167562-41-6P 167562-42-7P 167562-43-8P
167562-44-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of oligoamines as anticoagulants and platelet aggregation inhibitors)

RN 167562-38-1 CAPLUS

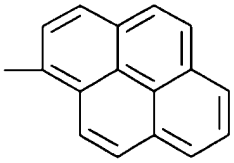
CN 1,2-Ethanediamine, N-(1-pyrenylmethyl)-N'-[2-[(1-pyrenylmethyl)amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

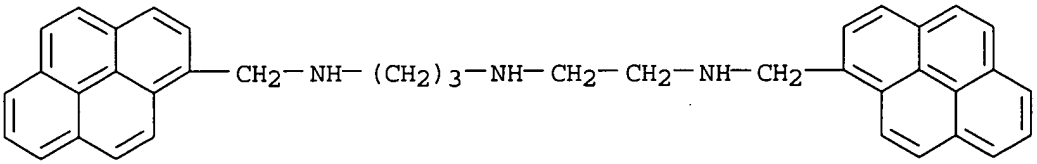


● 3 HCl

PAGE 1-B

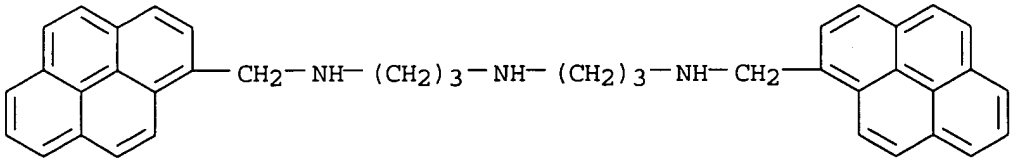


RN 167562-39-2 CAPLUS
CN 1,3-Propanediamine, N-(1-pyrenylmethyl)-N'-[2-[(1-pyrenylmethyl)amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)



● 3 HCl

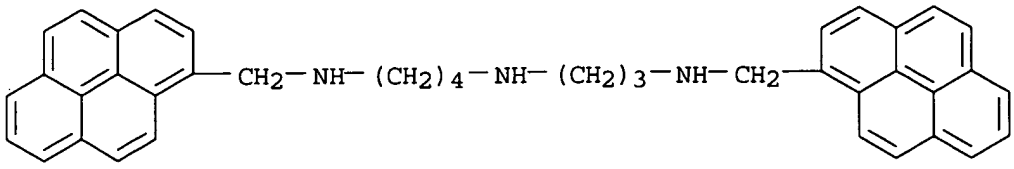
RN 167562-40-5 CAPLUS
CN 1,3-Propanediamine, N-(1-pyrenylmethyl)-N'-[3-[(1-pyrenylmethyl)amino]propyl]-, trihydrochloride (9CI) (CA INDEX NAME)



● 3 HCl

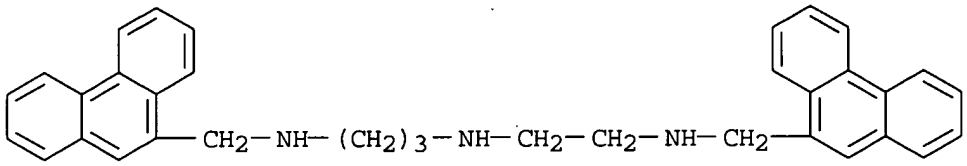
RN 167562-41-6 CAPLUS
CN 1,4-Butanediamine, N-(1-pyrenylmethyl)-N'-[3-[(1-

pyrenylmethyl)amino]propyl]-, trihydrochloride (9CI) (CA INDEX NAME)



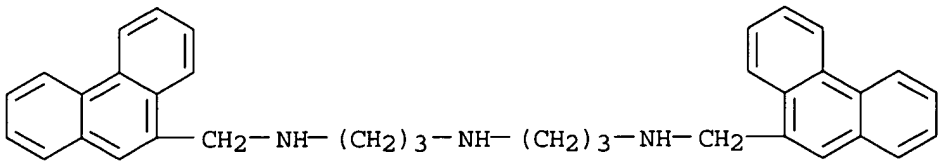
●3 HCl

RN 167562-42-7 CAPLUS
CN 1,3-Propanediamine, N-(9-phenanthrenylmethyl)-N'-[2-[(9-phenanthrenylmethyl)amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)



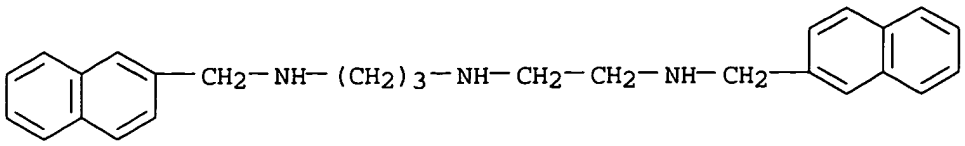
●3 HCl

RN 167562-43-8 CAPLUS
CN 1,3-Propanediamine, N-(9-phenanthrenylmethyl)-N'-[3-[(9-phenanthrenylmethyl)amino]propyl]-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

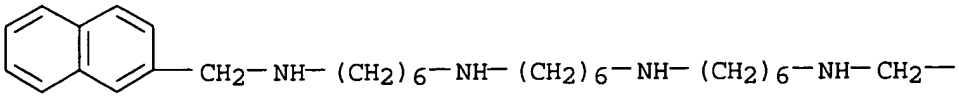
RN 167562-44-9 CAPLUS
CN 1,3-Propanediamine, N-(2-naphthalenylmethyl)-N'-[2-[(2-naphthalenylmethyl)amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

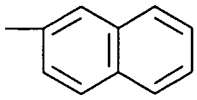
L15 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:457092 CAPLUS
DN 121:57092
TI Nonpeptide Peptidomimetic Antagonists of the Neuropeptide Y Receptor: Benextramine Analogs with Selectivity for the Peripheral Y2 Receptor
AU Chaurasia, Chandra; Misse, Gregory; Tessel, Richard; Doughty, Michael B.
CS Departments of Medicinal Chemistry and Pharmacology and Toxicology, University of Kansas, Lawrence, KS, 66045, USA
SO Journal of Medicinal Chemistry (1994), 37(14), 2242-8
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB A new series of benextramine analogs [RCH2NH(CH2)6XCH2CH2Y]2 [I; R = 2-naphthyl, 1-adamantyl, X = NH, NC(NH2):NH, Y = S, CH2] were prepared as neuropeptide Y (NPY) functional group mimetics and tested for N-[propionyl-3H]NPY ([3]NPY) displacement activity in rat brain membrane homogenates and for NPY receptor antagonist activity in the rat femoral artery. The tetraamine carbon analog I (R = 2-naphthyl, X = NH, Y = CH2) was equipotent with benextramine in a rat brain [3H]NPY displacement assay, suggesting that the disulfide is not a necessary feature of the benextramine activity, although this analog maintained selectivity for the benextramine-sensitive binding site population. Bis(N,N-dialkylguanyl) disulfide and carbon analogs I [R = 2-naphthyl, 1-adamantyl, X = NC(NH2):NH, Y = S, CH2] were 3-4 times more potent than their resp. controls in displacing [3H]NPY from rat brain membrane homogenates, and maintained selectivity for the benextramine-sensitive, Y1 binding site population. However, the activity of the carbon analog I.4HCl [R = 2-naphthyl, X = NC(NH2):NH, Y = CH2] showed a different profile in a femoral artery vasoconstriction assay; at 1.0 nM, this analog shifted the concentration-effect curve of the Y2-selective agonist NPY(13-36) to the right without a significant change in the maximum effect, while even at 1.0 mM it had no effect on the vasoconstrictive activity of the Y1-selective agonist [Leu31,Pro34]-NPY. Thus, the guanidino benextramine analogs I [X = NC(NH2):NH] are selective, competitive antagonists of the postsynaptic NPY receptor in the femoral artery.
IT **156272-83-2P 156272-84-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and neuropeptide Y antagonistic activity of)
RN 156272-83-2 CAPLUS
CN 1,6-Hexanediamine, N,N'-bis[6-[(2-naphthalenylmethyl)amino]-, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



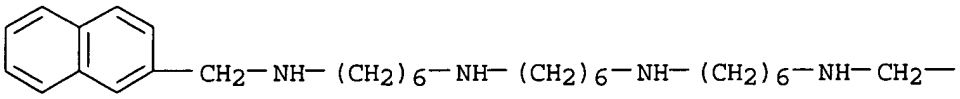
● 4 HCl

PAGE 1-B

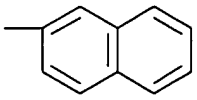


RN 156272-84-3 CAPLUS
CN 1,6-Hexanediamine, N,N'-bis[6-[(2-naphthalenylmethyl)amino]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L15 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:228377 CAPLUS
DN 114:228377
TI Preparation of polyazaalkenoic acids and analogs and their metal complexes for oxygen fixation
IN Boisselier-Cocolios, Brigitte; Guilard, Roger; Jean, Christophe; Taurin, Laurent
PA Air Liquide SA pour l'Etude et l'Exploitation des Procedes Georges Claude, Fr.
SO PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
PI	WO 9009987	A1	19900907	WO 1990-FR124		19900222
	W: AU, CA, JP, US					
				FR 1989-2315	A	19890222
	FR 2643370	A1	19900824	FR 1989-2315		19890222
	FR 2643370	B1	19910823			
	CA 2027578	AA	19900823	CA 1990-2027578		19900222
				FR 1989-2315	A	19890222
	AU 9051759	A1	19900926	AU 1990-51759		19900222
	AU 641142	B2	19930916			
				FR 1989-2315	A	19890222
				WO 1990-FR124	A	19900222
	EP 396435	A1	19901107	EP 1990-400488		19900222
	EP 396435	B1	19950621			
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE					
				FR 1989-2315	A	19890222
	ZA 9001363	A	19910327	ZA 1990-1363		19900222
				FR 1989-2315	A	19890222
	JP 03504134	T2	19910912	JP 1990-504238		19900222
				FR 1989-2315	A	19890222
				WO 1990-FR124	W	19900222
	US 6139603	A	20001031	US 1994-253233		19940602
				FR 1989-2315	A	19890222

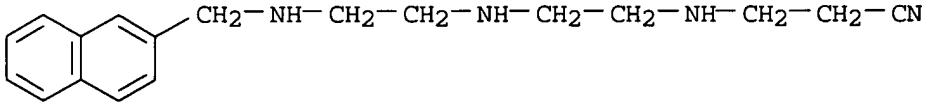
OS MARPAT 114:228377

AB The title compds., e.g., H[NH(CH2)2]4CO2H (I), H2N(CH2)3NH(CH2)2N(CH2CO2H)CH2CH2NH2, whose metal complexes are useful for fixation of oxygen and thus for anal. of oxygen, etc., are prepared via, e.g., addition of a polyazaalkane to acrylonitrile followed by hydrolysis, N-alkylation of hexahydro-5H-1,4-diazepine-5-one with an aminoalkyl halide followed by hydrolysis. Acrylonitrile was added to triethylenetetramine over 30 min, the formed blue solution stirred at ambient temperature for 24 h, excess triethylenetetramine removed by distillation under reduced pressure, and the obtained nitrile hydrolyzed with H2SO4 to give I. Co(II)[PhCH2(NHCH2CH2)3CO2H] was obtained by dissolving PhCH2(NHCH2CH2)3CO2H.2H2SO4.H2O in water, adjusting the solution to pH 7.47 and then, at complete dissoln., to pH 2.25 followed by treatment with Co(OAc)2.4H2O. Fixation of oxygen by the Co(II)[C6H5CH2(NHCH2CH2)3CO2H], obtained similarly, by forming the μ-peroxy complex LCoO2CoL (L = C6H5CH2(NHCH2)3CO2H] and recovering the oxygen by desorption is also demonstrated.

IT **133681-39-7P 133681-45-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 133681-39-7 CAPLUS

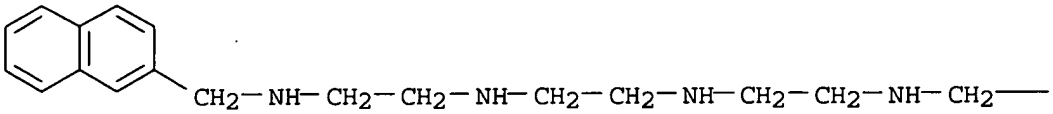
CN Propanenitrile, 3-[[2-[[2-[(2-naphthalenylmethyl)amino]ethyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)



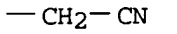
RN 133681-45-5 CAPLUS

CN 2,5,8,11-Tetraazatetradecane-14-nitrile, 1-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

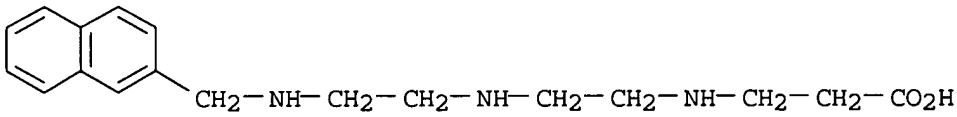
PAGE 1-A



PAGE 1-B

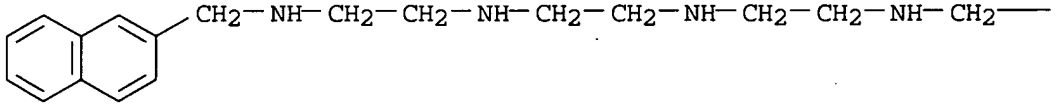


IT **133681-22-8P 133681-28-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for complexing with metals for oxygen fixation)
RN 133681-22-8 CAPLUS
CN β-Alanine, N-[2-[[2-[(2-naphthalenylmethyl)amino]ethyl]amino]ethyl]- (9CI) (CA INDEX NAME)

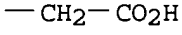


RN 133681-28-4 CAPLUS
CN 2,5,8,11-Tetraazatetradecan-14-oic acid, 1-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

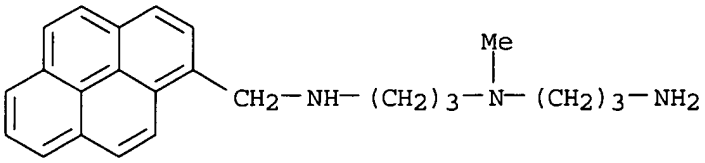


PAGE 1-B



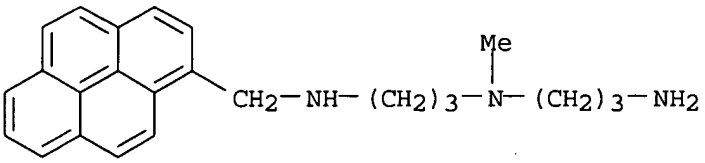
L15 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1990:514786 CAPLUS
DN 113:114786
TI [(1-Pyrenylmethyl)amino] alcohols, a new class of antitumor DNA intercalators. Discovery and initial amine side chain structure-activity studies.
AU Bair, Kenneth W.; Tuttle, Richard L.; Knick, Vincent C.; Cory, Michael; McKee, David D.
CS Div. Org. Chem., Burroughs Wellcome Co., Research Triangle Park, NC,

27709, USA
SO Journal of Medicinal Chemistry (1990), 33(9), 2385-93
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
OS CASREACT 113:114786
AB The relationships among structure, interaction with DNA, and murine antitumor activity of a series of 1-pyrenylmethylamines were examined Binding studies show that all 1-pyrenylmethylamine derivs. bind to some extent to DNA by intercalation. The presence of addnl. basic amine groups in the side chain enhances DNA binding due to electrostatic interactions. Compds. containing only a single basic benzylic amine bind similarly to DNA. Only the presence of bulky side chains decreases the DNA interactions. Although antitumor activity is seen for (1-pyrenylmethyl)amino alcs., useful antitumor activity in the series is limited to congeners bearing the 2-amino-1,3-propanediol side chain. These derivs. bind moderately to DNA. DNA binding is a necessary but not sufficient criterion for antitumor activity. In addition, the strength of DNA binding does not correlate with the antitumor activity.
IT **127856-54-6P 127856-55-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, DNA binding, and murine antitumor activity of)
RN 127856-54-6 CAPLUS
CN 1,3-Propanediamine, N-(3-aminopropyl)-N-methyl-N'-(1-pyrenylmethyl)-, trihydrochloride (9CI) (CA INDEX NAME)



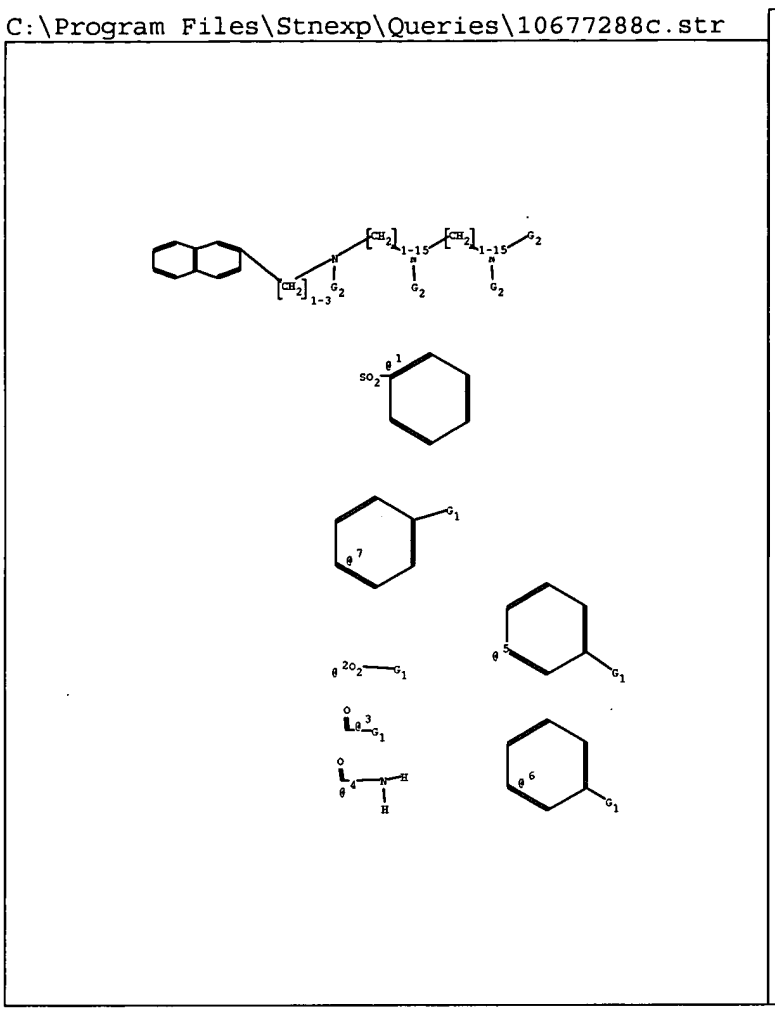
●3 HCl

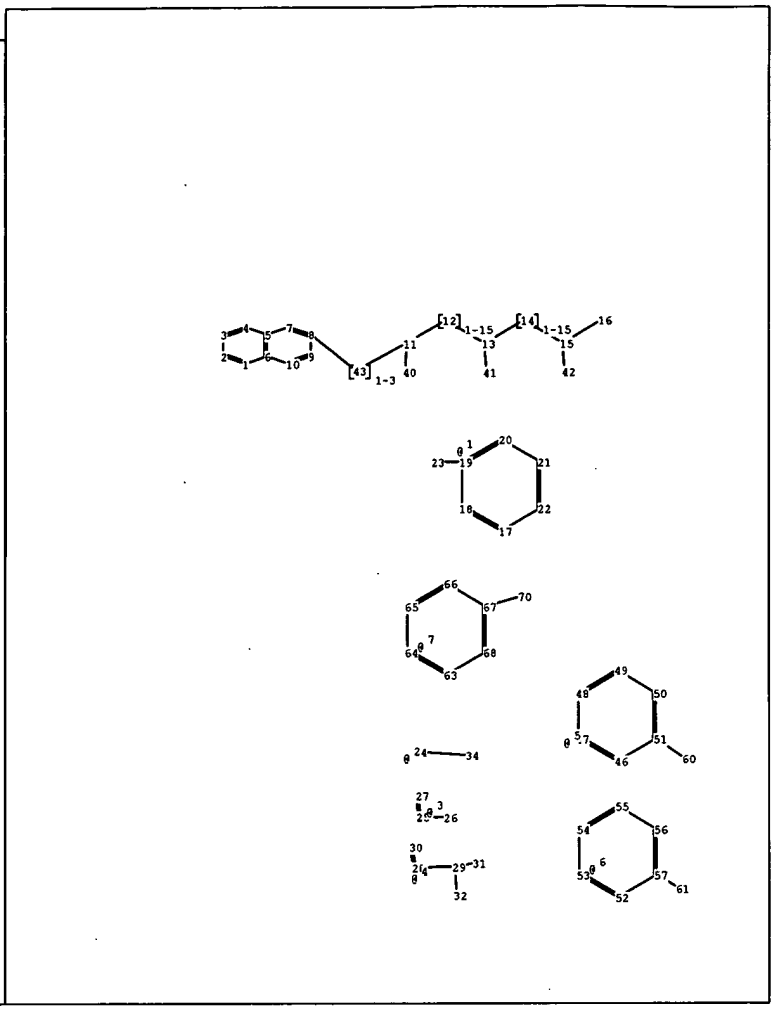
RN 127856-55-7 CAPLUS
CN 1,3-Propanediamine, N-(3-aminopropyl)-N-methyl-N'-(1-pyrenylmethyl)- (9CI) (CA INDEX NAME)



=>

C:\Program Files\Stnexp\Queries\10677288c.str





chain nodes :
11 12 13 14 15 16 23 24 25 26 27 28 29 30 31 32 34 40 41 42 43 60
61 70
ring nodes :
1 2 3 4 5 6 7 8 9 10 17 18 19 20 21 22 46 47 48 49 50 51 52 53 54
55 56 57 63 64 65 66 67 68
chain bonds :
8-43 11-12 11-40 11-43 12-13 13-14 13-41 14-15 15-16 15-42 19-23 24-34 25-26
25-27 28-29 28-30 29-31 29-32 51-60 57-61 67-70
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 17-18 17-22 18-19 19-20
20-21 21-22 46-47 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56
56-57 63-64 63-68 64-65 65-66 66-67 67-68
exact/norm bonds :
11-40 13-41 15-16 15-42 24-34 25-26 25-27 28-29 28-30 51-60 57-61 67-70
exact bonds :
8-43 11-12 11-43 12-13 13-14 14-15 19-23 29-31 29-32
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 17-18 17-22 18-19 19-20
20-21 21-22 46-47 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56
56-57 63-64 63-68 64-65 65-66 66-67 67-68

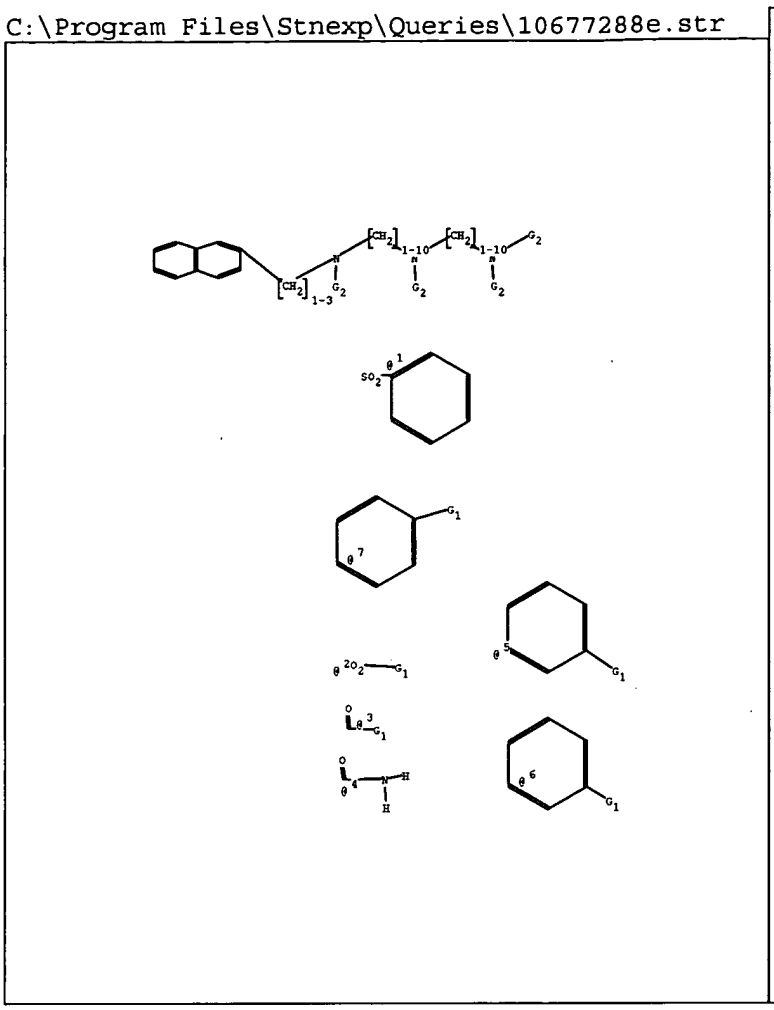
G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

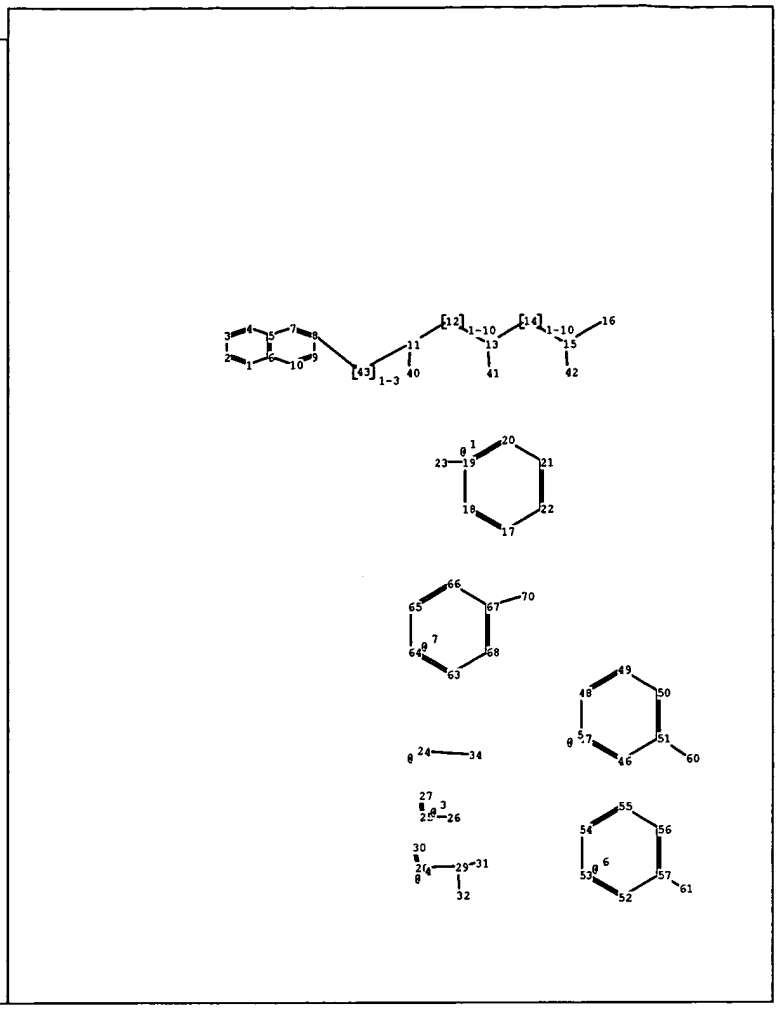
G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom

34:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 60:Atom
61:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom

C:\Program Files\Stnexp\Queries\10677288e.str





chain nodes :
11 12 13 14 15 16 23 24 25 26 27 28 29 30 31 32 34 40 41 42 43 60
61 70
ring nodes :
1 2 3 4 5 6 7 8 9 10 17 18 19 20 21 22 46 47 48 49 50 51 52 53 54
55 56 57 63 64 65 66 67 68
chain bonds :
8-43 11-12 11-40 11-43 12-13 13-14 13-41 14-15 15-16 15-42 19-23 24-34 25-26
25-27 28-29 28-30 29-31 29-32 51-60 57-61 67-70
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 17-18 17-22 18-19 19-20
20-21 21-22 46-47 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56
56-57 63-64 63-68 64-65 65-66 66-67 67-68
exact/norm bonds :
11-40 13-41 15-16 15-42 24-34 25-26 25-27 28-29 28-30 51-60 57-61 67-70
exact bonds :
8-43 11-12 11-43 12-13 13-14 14-15 19-23 29-31 29-32
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 17-18 17-22 18-19 19-20
20-21 21-22 46-47 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56
56-57 63-64 63-68 64-65 65-66 66-67 67-68

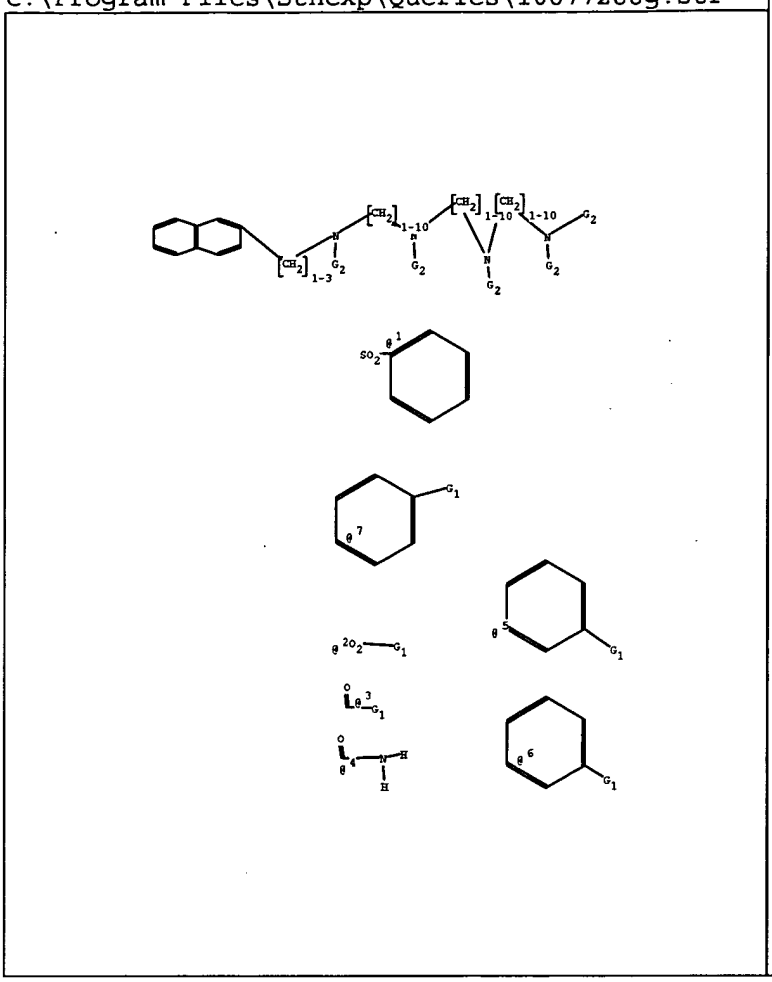
G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

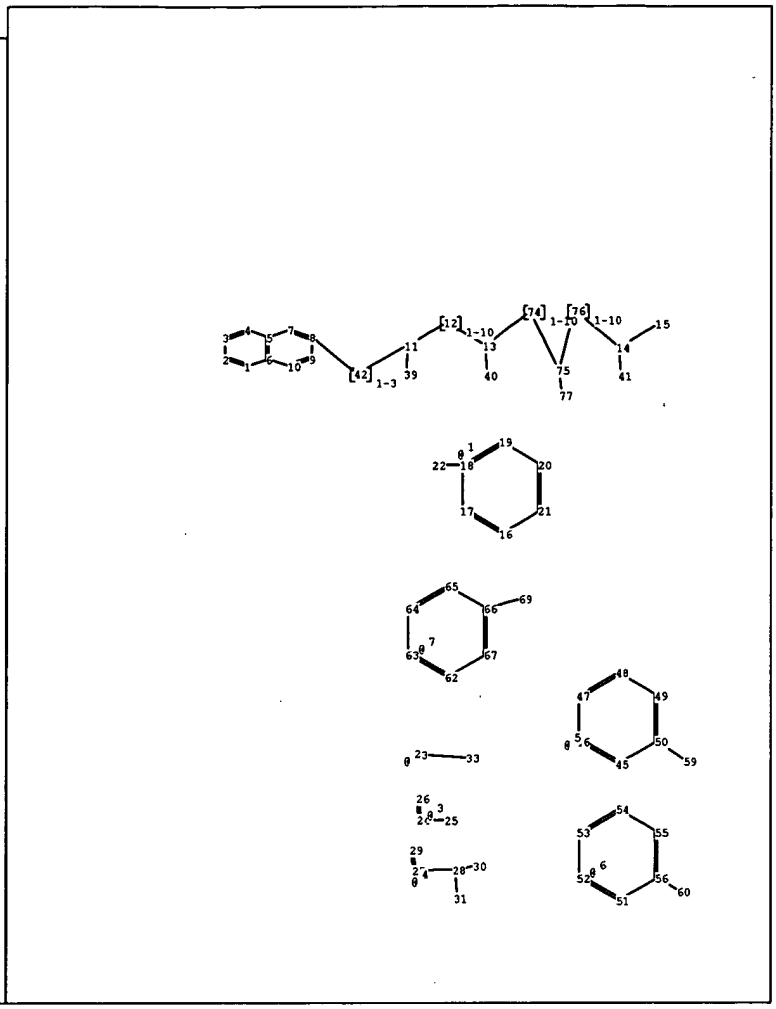
G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom

34:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 60:Atom
61:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom

C:\Program Files\Stnexp\Queries\10677288g.str





chain nodes :
11 12 13 14 15 22 23 24 25 26 27 28 29 30 31 33 39 40 41 42 59 60
69 74 75 76 77
ring nodes :
1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 45 46 47 48 49 50 51 52 53
54 55 56 62 63 64 65 66 67
chain bonds :
8-42 11-12 11-39 11-42 12-13 13-40 13-74 14-41 14-15 14-76 18-22 23-33 24-25
24-26 27-28 27-29 28-30 28-31 50-59 56-60 66-69 74-75 75-76 75-77
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55
55-56 62-63 62-67 63-64 64-65 65-66 66-67
exact/norm bonds :
11-39 13-40 14-41 14-15 23-33 24-25 24-26 27-28 27-29 50-59 56-60 66-69 75-77
exact bonds :
8-42 11-12 11-42 12-13 13-74 14-76 18-22 28-30 28-31 74-75 75-76
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55
55-56 62-63 62-67 63-64 64-65 65-66 66-67

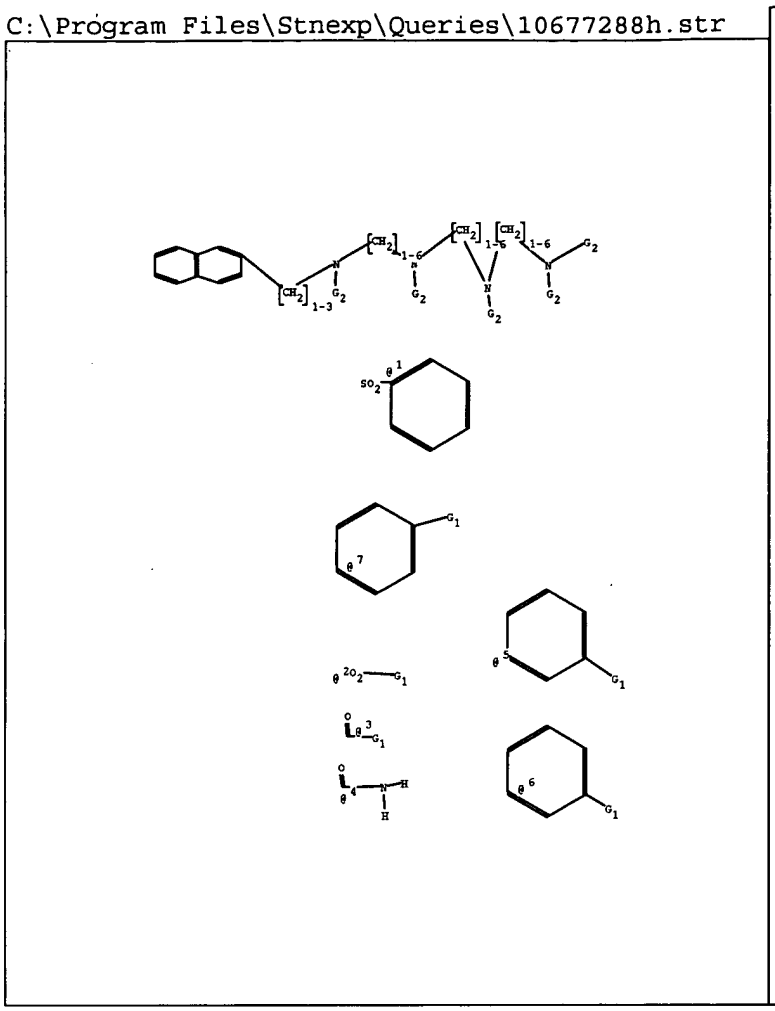
G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

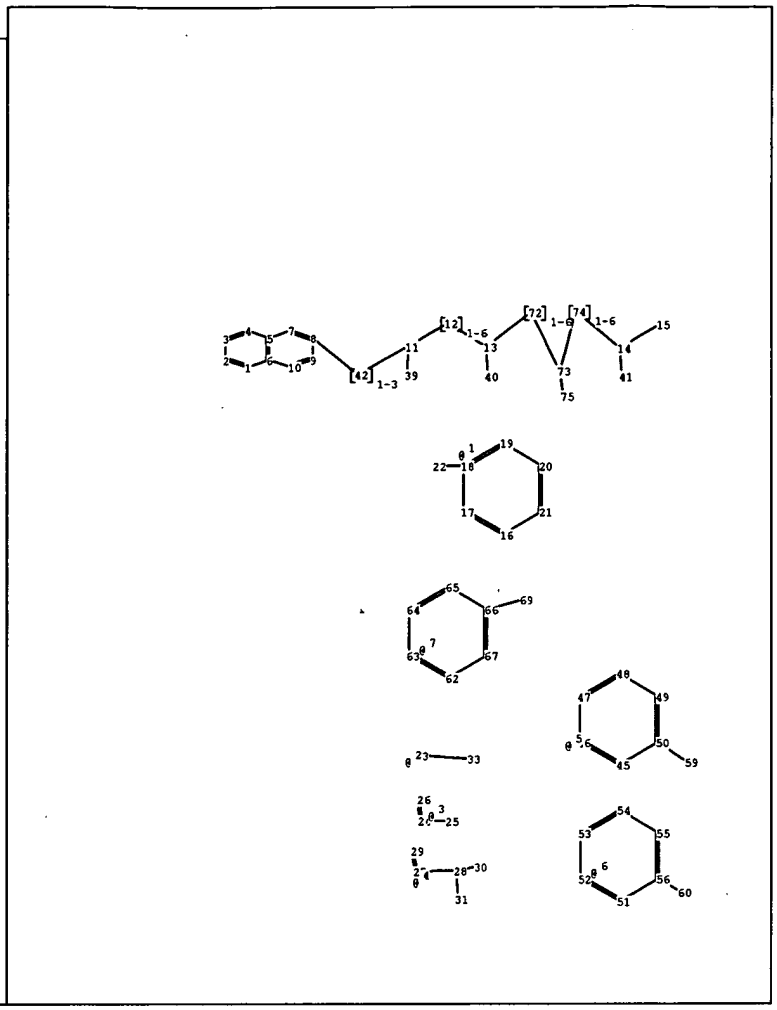
G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
33:Atom

39:CLASS 40:CLASS 41:CLASS 42:CLASS 45:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 59:Atom 60:Atom
62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:Atom 74:CLASS 75:CLASS
76:CLASS 77:CLASS

C:\Program Files\Stnexp\Queries\10677288h.str





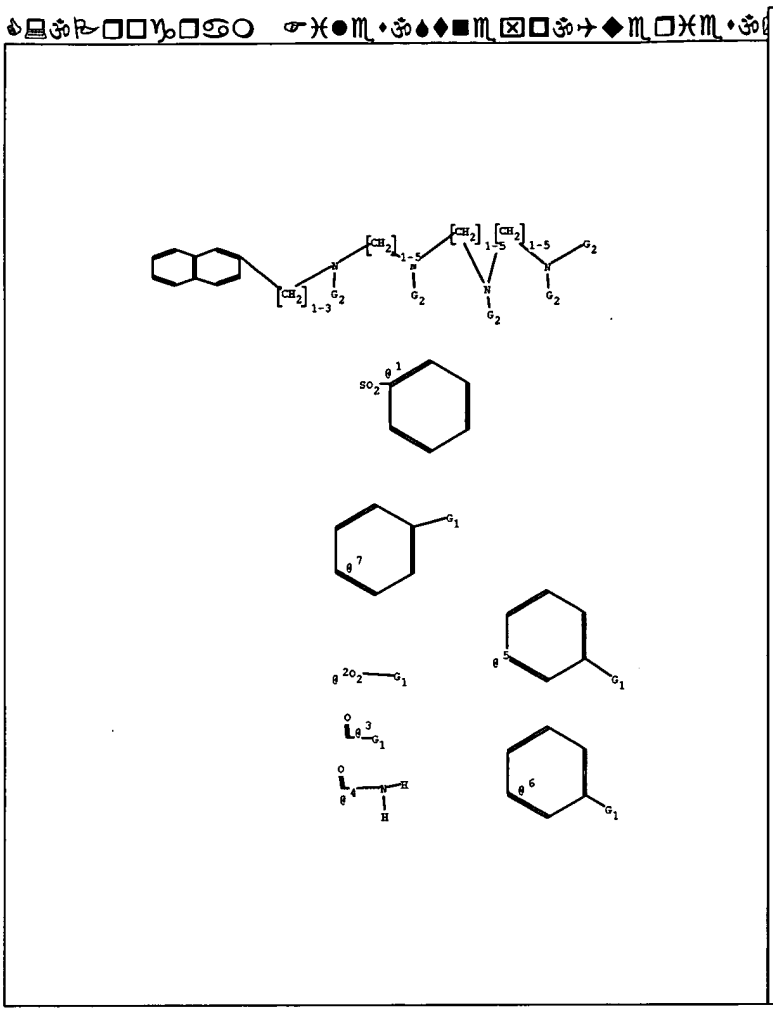
chain nodes :
11 12 13 14 15 22 23 24 25 26 27 28 29 30 31 33 39 40 41 42 59 60
69 72 73 74 75
ring nodes :
1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 45 46 47 48 49 50 51 52 53
54 55 56 62 63 64 65 66 67
chain bonds :
8-42 11-12 11-39 11-42 12-13 13-40 13-72 14-41 14-15 14-74 18-22 23-33 24-25
24-26 27-28 27-29 28-30 28-31 50-59 56-60 66-69 72-73 73-74 73-75
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55
55-56 62-63 62-67 63-64 64-65 65-66 66-67
exact/norm bonds :
11-39 13-40 14-41 14-15 23-33 24-25 24-26 27-28 27-29 50-59 56-60 66-69 73-75
exact bonds :
8-42 11-12 11-42 12-13 13-72 14-74 18-22 28-30 28-31 72-73 73-74
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55
55-56 62-63 62-67 63-64 64-65 65-66 66-67

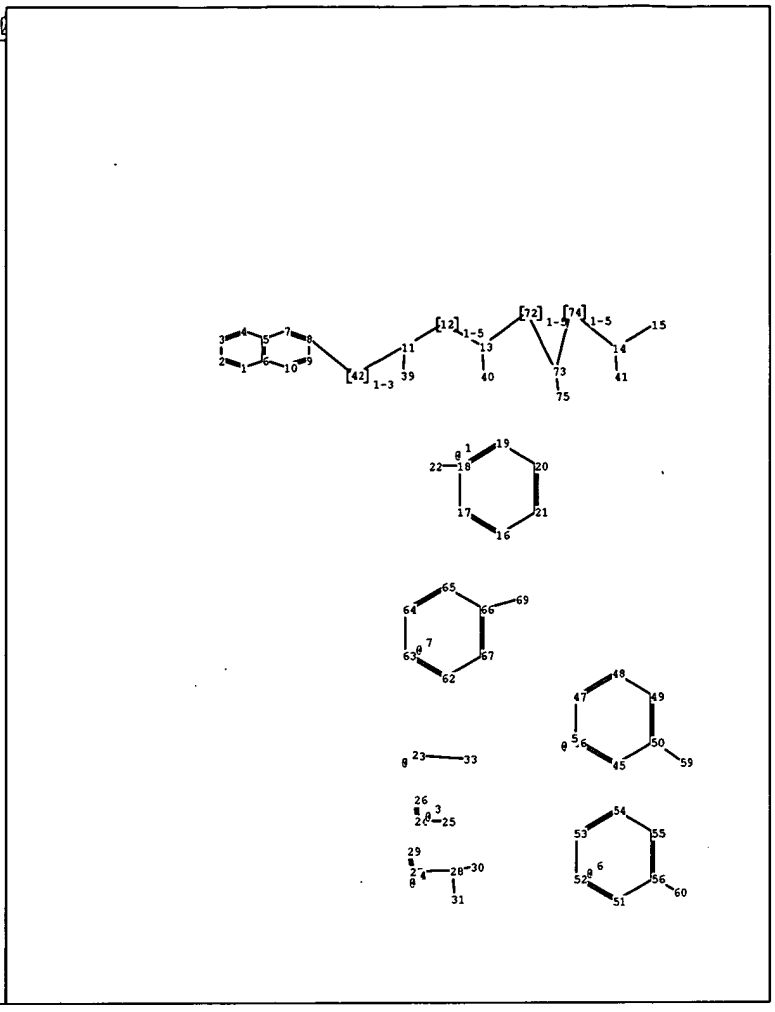
G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
33:Atom

39:CLASS 40:CLASS 41:CLASS 42:CLASS 45:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 59:Atom 60:Atom
62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:Atom 72:CLASS 73:CLASS
74:CLASS 75:CLASS



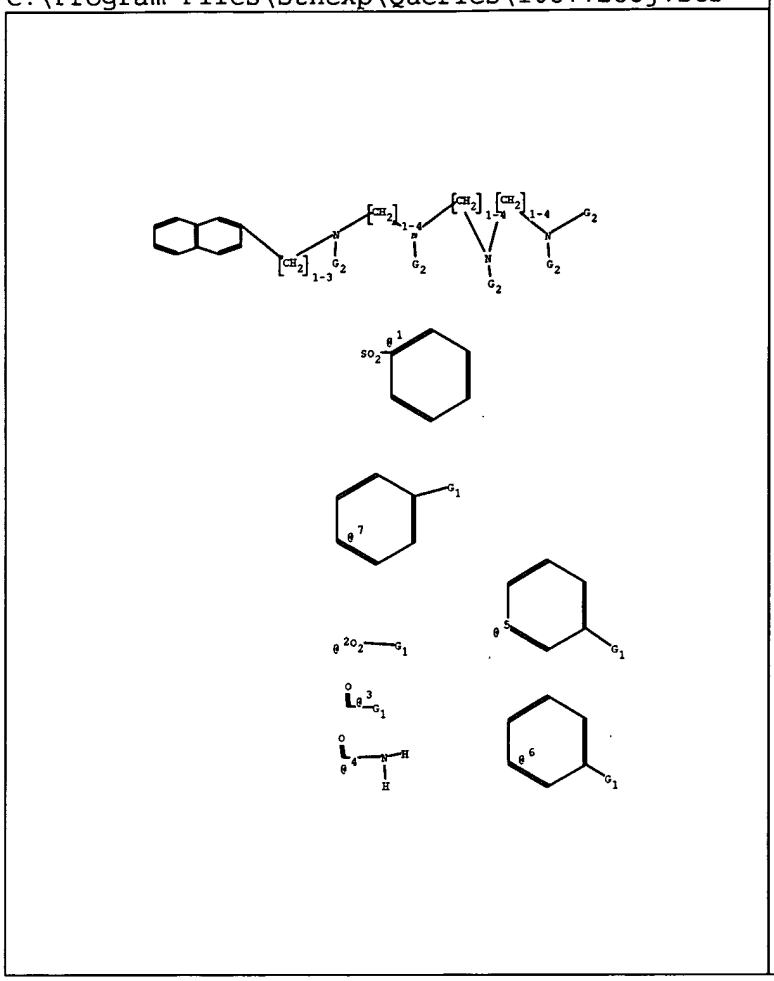


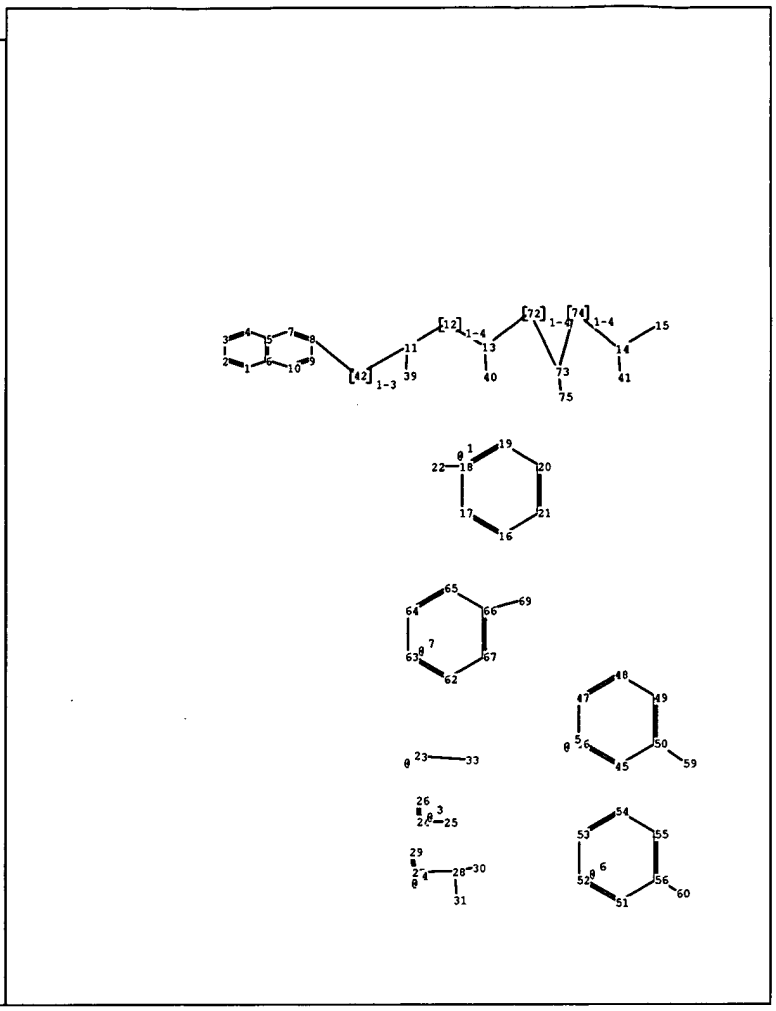
🖮☸

💣*♋♦♍♒ ●♏❖♏● 💻

📂💻✌♦□❍ 🗋💻✌♦□❍ 🗏💻✌♦□❍ 🗐💻✌♦□❍ 🗄💻✌♦□❍ ⌛💻✌♦□❍ 🖮💻✌♦□❍
🖰💻✌♦□❍ 🖲💻✌♦□❍ 📂🗀💻✌♦□❍ 📂📂💻✌♦□❍ 📂🗋💻✌♦□❍ 📂🗏💻✌♦□❍
📂🗐💻✌♦□❍ 📂🗄💻👍☹✌💧💧 📂⌛💻✌♦□❍ 📂🖮💻✌♦□❍ 📂🖰💻✌♦□❍ 📂🖲💻✌♦□❍
🗋🗀💻✌♦□❍ 🗋📂💻✌♦□❍ 🗋🗋💻✌♦□❍ 🗋🗏💻👍☹✌💧💧 🗋🗐💻✌♦□❍ 🗋🗄💻✌♦□❍
🗋⌛💻✌♦□❍ 🗋🖮💻✌♦□❍ 🗋🖰💻✌♦□❍ 🗋🖲💻✌♦□❍ 🗏🗀💻✌♦□❍ 🗏📂💻✌♦□❍
🗏🗏💻✌♦□❍ 🗏🖲💻👍☹✌💧💧 🗐🗀💻👍☹✌💧💧 🗐📂💻👍☹✌💧💧 🗐🗋💻👍☹✌💧💧 🗐🗄💻✌♦□❍
🗐⌛💻✌♦□❍ 🗐🖮💻✌♦□❍ 🗐🖰💻✌♦□❍ 🗐🖲💻✌♦□❍ 🗄🗀💻✌♦□❍ 🗄📂💻✌♦□❍
🗄🗋💻✌♦□❍ 🗄🗏💻✌♦□❍ 🗄🗐💻✌♦□❍ 🗄🗄💻✌♦□❍ 🗄⌛💻✌♦□❍ 🗄🖲💻✌♦□❍
⌛🗀💻✌♦□❍ ⌛🗋💻✌♦□❍ ⌛🗏💻✌♦□❍ ⌛🗐💻✌♦□❍ ⌛🗄💻✌♦□❍ ⌛⌛💻✌♦□❍
⌛🖮💻✌♦□❍ ⌛🖲💻✌♦□❍ 🖮🗋💻👍☹✌💧💧 🖮🗏💻👍☹✌💧💧 🖮🗐💻👍☹✌💧💧 🖮🗄💻👍☹✌💧💧

C:\Program Files\Stnexp\Queries\10677288j.str





chain nodes :
11 12 13 14 15 22 23 24 25 26 27 28 29 30 31 33 39 40 41 42 59 60
69 72 73 74 75
ring nodes :
1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 45 46 47 48 49 50 51 52 53
54 55 56 62 63 64 65 66 67
chain bonds :
8-42 11-12 11-39 11-42 12-13 13-40 13-72 14-41 14-15 14-74 18-22 23-33 24-25
24-26 27-28 27-29 28-30 28-31 50-59 56-60 66-69 72-73 73-74 73-75
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55
55-56 62-63 62-67 63-64 64-65 65-66 66-67
exact/norm bonds :
11-39 13-40 14-41 14-15 23-33 24-25 24-26 27-28 27-29 50-59 56-60 66-69 73-75
exact bonds :
8-42 11-12 11-42 12-13 13-72 14-74 18-22 28-30 28-31 72-73 73-74
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55
55-56 62-63 62-67 63-64 64-65 65-66 66-67

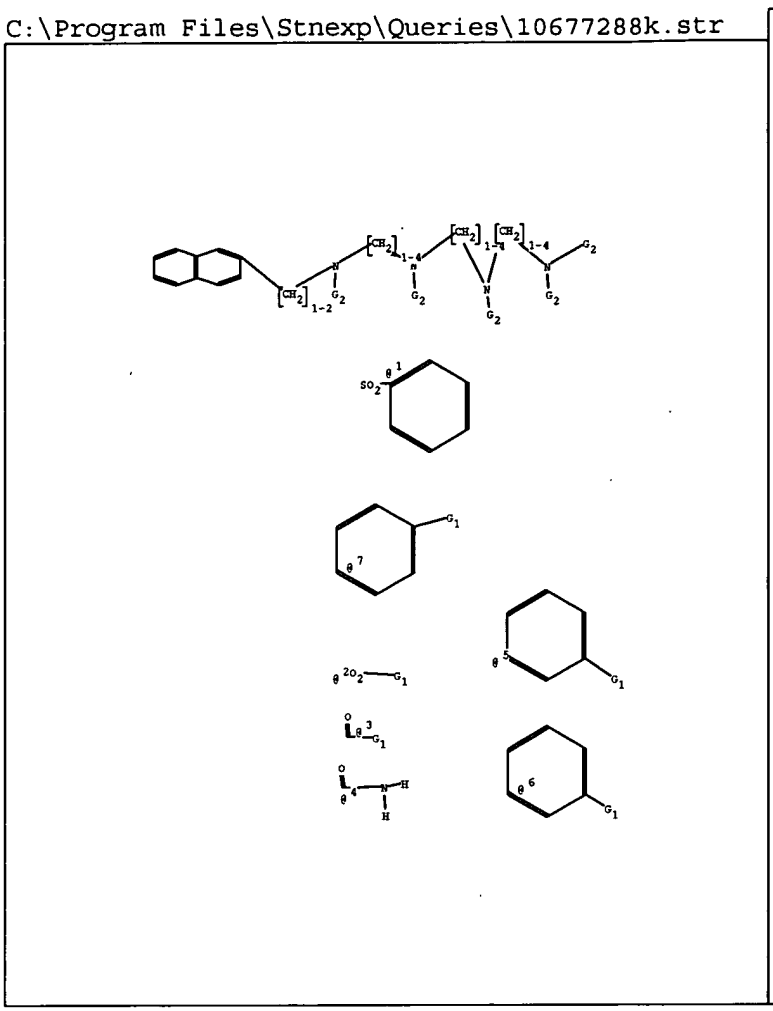
G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

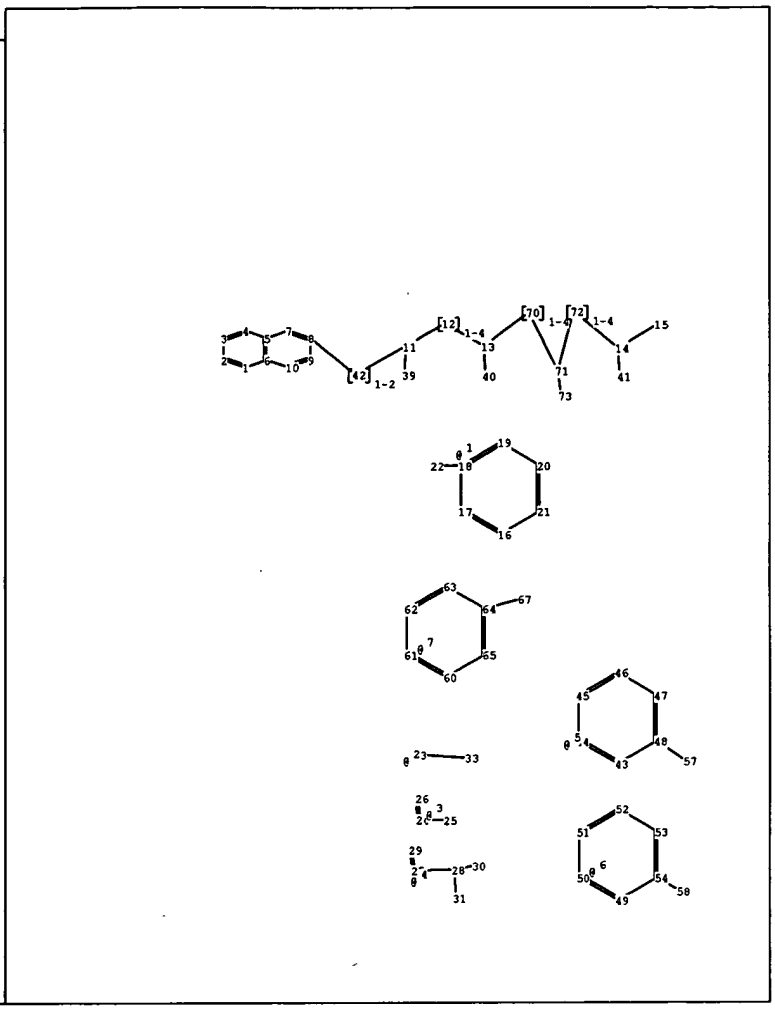
G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
33:Atom

39:CLASS 40:CLASS 41:CLASS 42:CLASS 45:Atom 46:Atom 47:Atom 48:Atom
49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 59:Atom 60:Atom
62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:Atom 72:CLASS 73:CLASS
74:CLASS 75:CLASS

C:\Program Files\Stnexp\Queries\10677288k.str





chain nodes :
11 12 13 14 15 22 23 24 25 26 27 28 29 30 31 33 39 40 41 42 57 58
67 70 71 72 73
ring nodes :
1 2 3 4 5 6 7 8 9 10 16 17 18 19 20 21 43 44 45 46 47 48 49 50 51
52 53 54 60 61 62 63 64 65
chain bonds :
8-42 11-12 11-39 11-42 12-13 13-40 13-70 14-41 14-15 14-72 18-22 23-33 24-25
24-26 27-28 27-29 28-30 28-31 48-57 54-58 64-67 70-71 71-72 71-73
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21 43-44 43-48 44-45 45-46 46-47 47-48 49-50 49-54 50-51 51-52 52-53
53-54 60-61 60-65 61-62 62-63 63-64 64-65
exact/norm bonds :
11-39 13-40 14-41 14-15 23-33 24-25 24-26 27-28 27-29 48-57 54-58 64-67 71-73
exact bonds :
8-42 11-12 11-42 12-13 13-70 14-72 18-22 28-30 28-31 70-71 71-72
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21 43-44 43-48 44-45 45-46 46-47 47-48 49-50 49-54 50-51 51-52 52-53
53-54 60-61 60-65 61-62 62-63 63-64 64-65

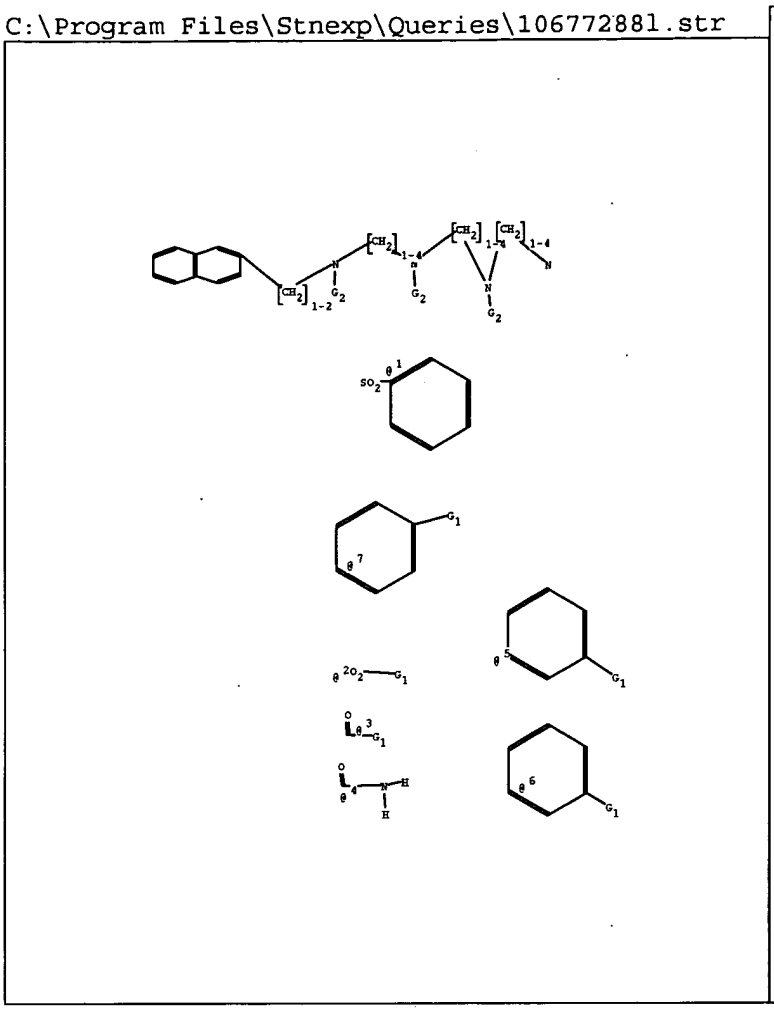
G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

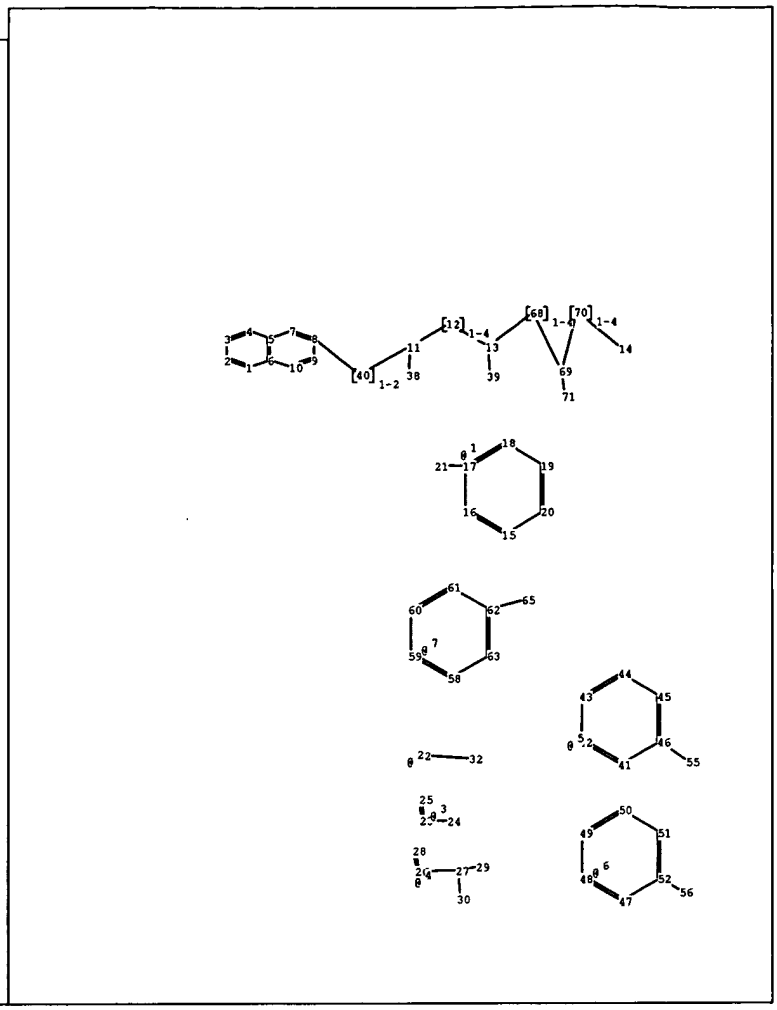
G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
33:Atom

39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:Atom 44:Atom 45:Atom 46:Atom
47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 57:Atom 58:Atom
60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom 67:Atom 70:CLASS 71:CLASS
72:CLASS 73:CLASS

C:\Program Files\Stnexp\Queries\10677288l.str





chain nodes :
11 12 13 14 21 22 23 24 25 26 27 28 29 30 32 38 39 40 55 56 65 68
69 70 71
ring nodes :
1 2 3 4 5 6 7 8 9 10 15 16 17 18 19 20 41 42 43 44 45 46 47 48 49
50 51 52 58 59 60 61 62 63
chain bonds :
8-40 11-12 11-38 11-40 12-13 13-39 13-68 14-70 17-21 22-32 23-24 23-25 26-27
26-28 27-29 27-30 46-55 52-56 62-65 68-69 69-70 69-71
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 15-16 15-20 16-17 17-18
18-19 19-20 41-42 41-46 42-43 43-44 44-45 45-46 47-48 47-52 48-49 49-50 50-51
51-52 58-59 58-63 59-60 60-61 61-62 62-63
exact/norm bonds :
11-38 13-39 22-32 23-24 23-25 26-27 26-28 46-55 52-56 62-65 69-71
exact bonds :
8-40 11-12 11-40 12-13 13-68 14-70 17-21 27-29 27-30 68-69 69-70
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 15-16 15-20 16-17 17-18
18-19 19-20 41-42 41-46 42-43 43-44 44-45 45-46 47-48 47-52 48-49 49-50 50-51
51-52 58-59 58-63 59-60 60-61 61-62 62-63

G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 32:Atom
38:CLASS

39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom
47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 55:Atom 56:Atom 58:Atom 59:Atom
60:Atom 61:Atom 62:Atom 63:Atom 65:Atom 68:CLASS 69:CLASS 70:CLASS 71:CLASS